

CPU

GPU

Grid generation

**a** Position and group  
for each point

**c** Significant functions  
for each group

**b** Points weight

**d** Starting guess

**e** Precompute ERIs  
and QM/MM

Density matrix

Kohn-Sham matrix construction

**f** ERIs

**g** One electron

**h** QM/MM

Exchange and correlation

For each point:

**i** Function values

**j** Density and derivs

**k** K-S matrix elements

**l** Fock matrix diagonalization

Output: Wave function  
and energy

Until SCF convergence

